High Performance Computing

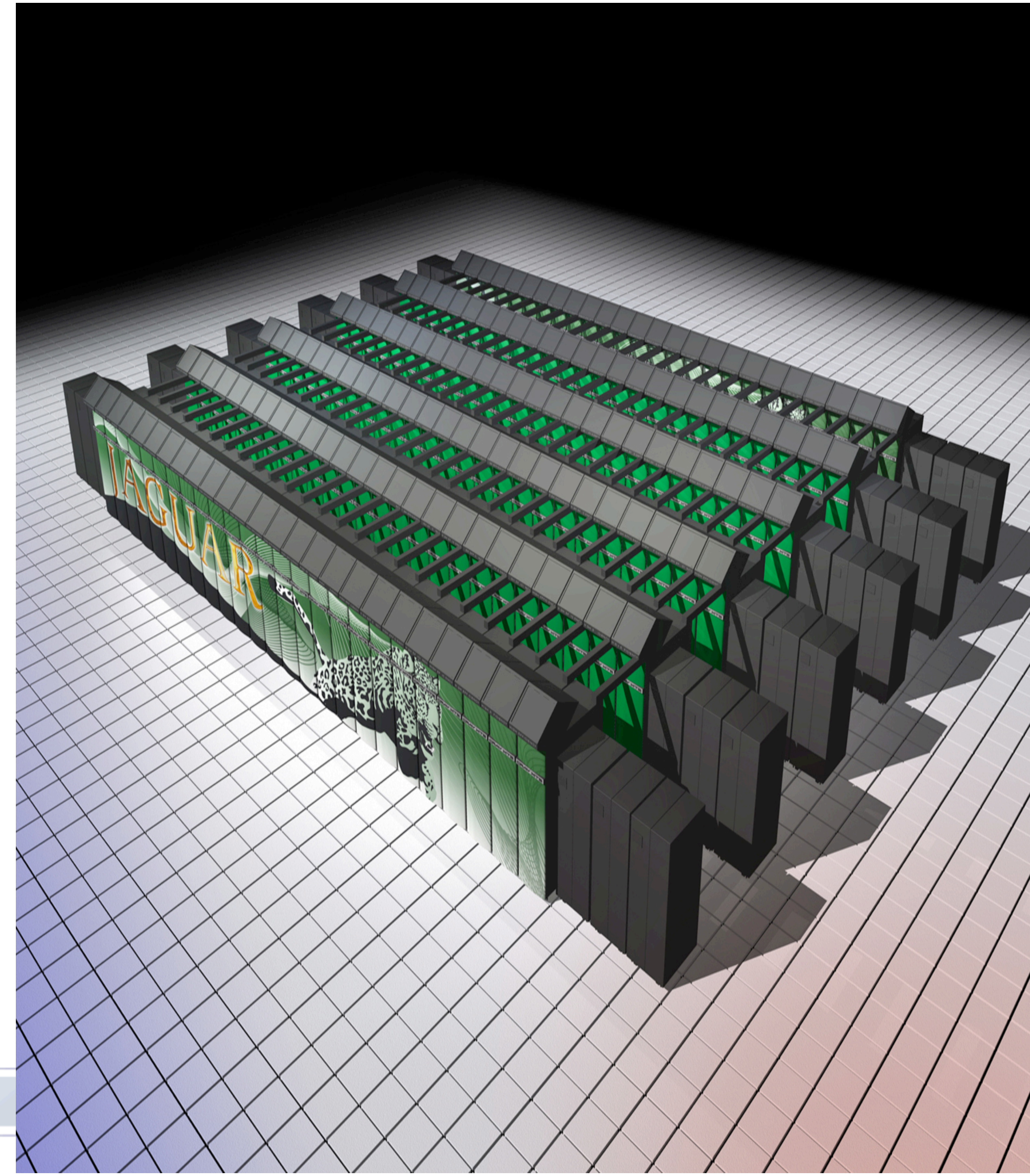
NATIONAL CENTER
FOR COMPUTATIONAL SCIENCES

Robert Whitten Jr

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Welcome!

- Today's Agenda:
  - Introduction
  - What is HPC?
  - Course Overview
  - Getting accounts



Instructor introduction

- Robert Whitten Jr. (Bobby)
- Computer Scientist / Software Engineer
- HPC User Support Specialist with NCCS at ORNL
- Scuba instructor / underwater cave diver

Introduction to course

- Video-based teleconference course
- Instructed through joint efforts between university and Oak Ridge National Laboratory
- Survey course covering HPC topics
  - Unix/linux
  - Parallel programming
  - Model design
  - Parallel I/O
  - Visualization

What is HPC?

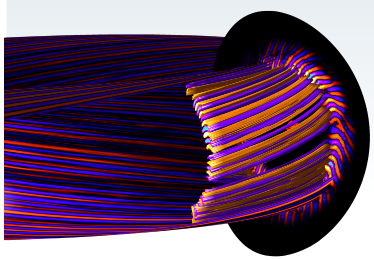
- High Performance Computing (HPC)
  - aka Supercomputing
  - aka High End Computing (HEC)
  - aka Cyberinfrastructure (CI)
- Biggest, fastest computing resource right this minute
  - aka Supercomputers

Why HPC? = Science drivers

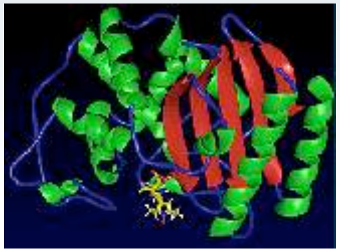
"Computational simulation offers to enhance, as well as leapfrog, theoretical and experimental progress in many areas of science and engineering…"

A Science-Based Case for Large-Scale Simulation (SCaLeS Report), Office of Science, U.S. DOE, July 2003

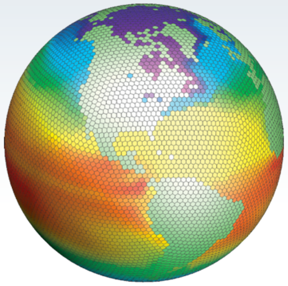
Advanced energy systems
- Fuel cells
- Fusion



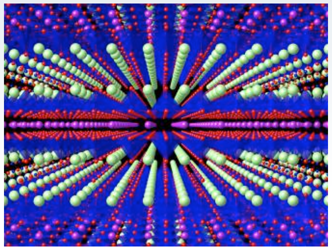
Biotechnology
- Genomics
- Cellular dynamics



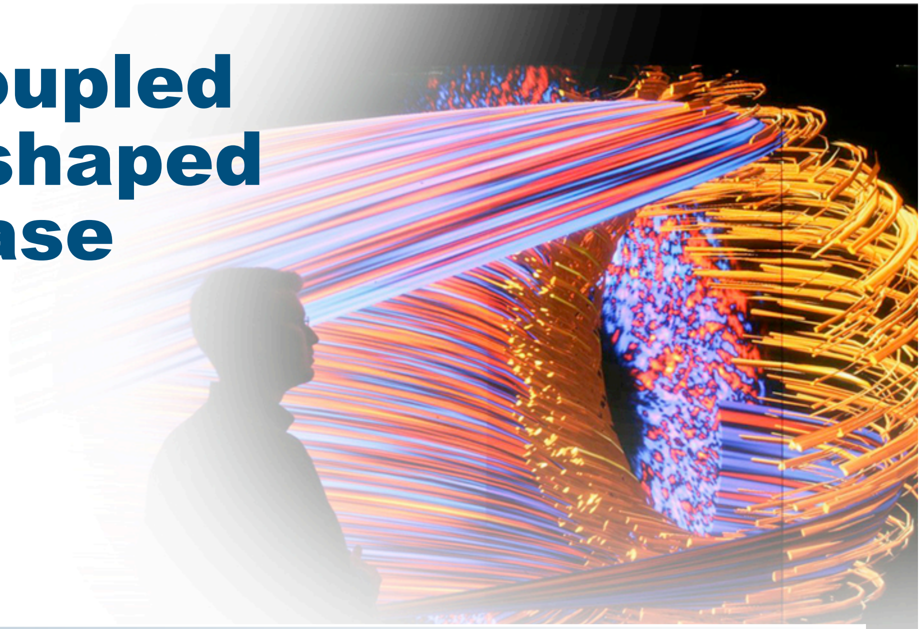
Environmental modeling
- Climate prediction
- Pollution remediation



Nanotechnology
- Sensors
- Storage devices



New ability to model coupled ETG/ITG turbulence in shaped plasma in nonlinear phase



Impact: Modeling and understanding of plasma turbulence is crucial for development of stable and efficient fusion devices

Problem:

- Computational modeling of interaction of turbulence on ion and electron spatial and temporal scales
- Scales differ by orders of magnitude and have traditionally been treated by separate simulations

Results:
Simulations shed new light on how short-wavelength ETG turbulence comes into play as long-wavelength (ITG/TEM) turbulence is suppressed in pedestal (an edge transport barrier)

Ron Waltz, General Atomics

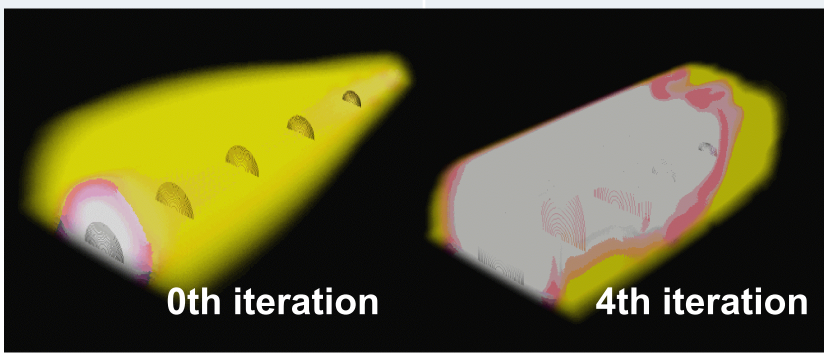
Fusion plasma:
Evolution of nonthermal plasma distributions during ion cyclotron resonance heating

Interaction of radio -frequency (RF) waves with fusion alpha particles must be understood and optimized for successful power production

Increasing current knowledge will help to plan and analyze ITER experiments

Self-consistent simulations of energetic ion evolution in plasma heated by RF waves in the ion cyclotron range of frequencies (ICRF) have been carried out on the LCF systems

Using the AORSA code coupled to the CQL3D Fokker-Planck code, we can now simulate evolution of ion distributions during ICRF heating

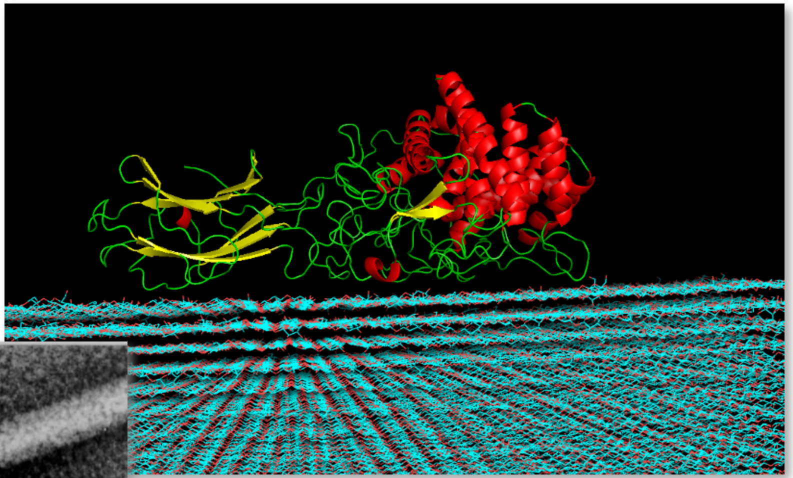


Bounce-averaged minority hydrogen distribution function in Alcator C-MOD shot 1051206002 at f = 80 MHz

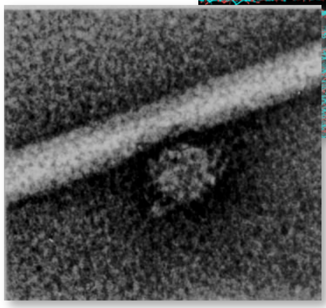
Don Batchelor, Oak Ridge National Laboratory

Creation of efficient enzymes for cellulose degradation through protein engineering

- **Renewable energy**: Ethanol production from cellulose
- Developing a detailed understanding of cellulase enzyme mechanisms from multiscale modeling
  - 1- to 100-ns trajectories for systems with more than 800,000 atoms
- Carrying out simulations with different substrates and mutant enzymes



Metabolism of cellulose by exocellulase enzyme



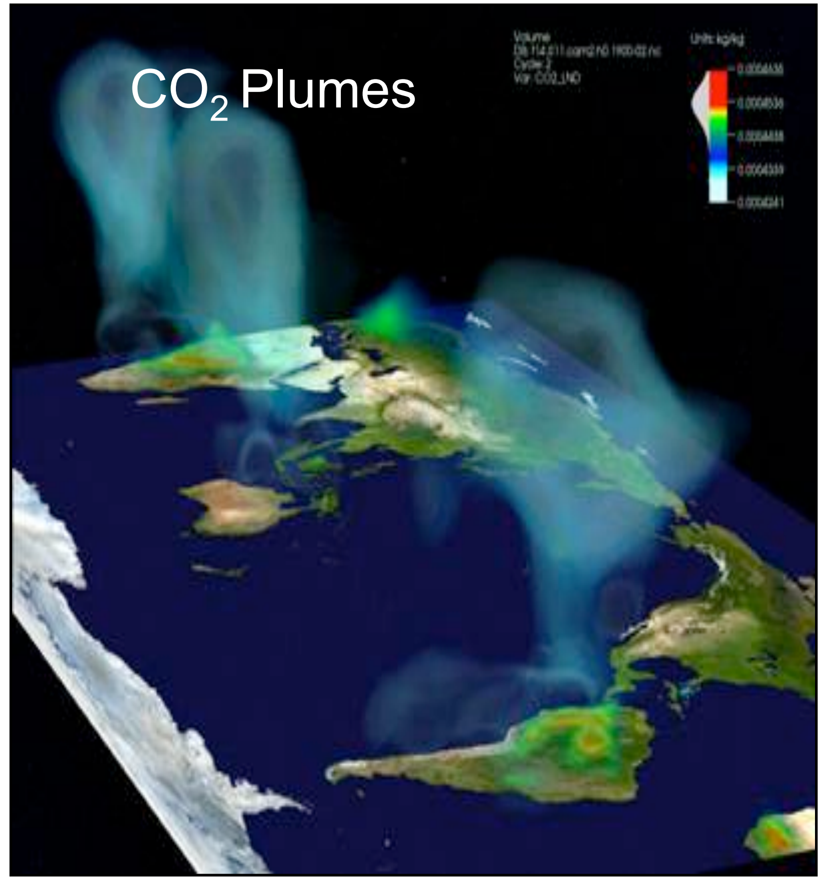
C. thermocellum growing on cellulose

Pratul Agarwal, Oak Ridge National Laboratory

Firsts in global climate modeling

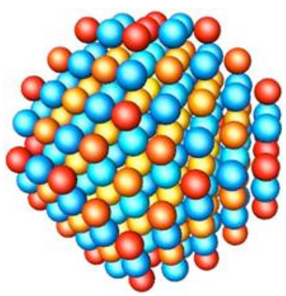
Results from model advances:

- First series of equilibration runs for Carbon Land-Model Intercomparison Project (C-LAMP)
- First-ever CCSM validation with new finite-volume dynamical core (FV dycore): Critical for chemistry and full carbon cycle
- Completed first 300-year run
- Four ensemble runs with natural CO_2 forcing
- Four new ensemble runs started for anthropogenic forcing
- New results from equilibrium runs of CASA′ and CN carbon-cycle models



Warren Washington, National Center for Atmospheric Research

Insight into next-generation recording media: Magnetic properties of FePt nanoparticles

FePt magnetic nanoparticles	Highly optimized calculations on LCF	Summary of results
• Material identified by industry for next-generation magnetic recording (>1 Tb psi) 	• DFT calculations using codes optimized with Cray Center of Excellence • Largest, most complex calculations of this type to date • ~50% of peak on 512 Jaguar processors (1 TF) for ~800 atoms • 2000 atoms planned	• Revealed, for first time, strong influence of nanoscale on magnetic structure of FePt nanoparticles • Sensitivity of magnetic structure to small changes demonstrates importance of calculations for materials design and optimization 

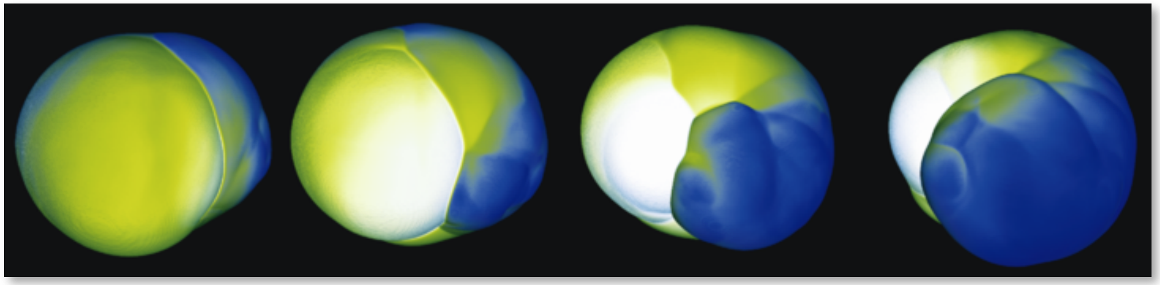
Thomas Schulthess, Oak Ridge National Laboratory

Evolution of supernovae

Supernova models must incorporate all known physics (in spite of computational demands) to capture phenomena

- **Explosions were obtained for 11 and 15 solar mass progenitors**
- **Explosions seem to be contingent on simulating all of:**
  - Multidimensional hydro
  - Good transport (MGFLD)
  - Nuclear burning
  - Long physical times (equivalent to long run times)

- **Researchers were surprised to find that nuclear burning has an important dynamic effect**
- **New result builds on earlier SASI findings**
  - Longer time scales required to observe explosion



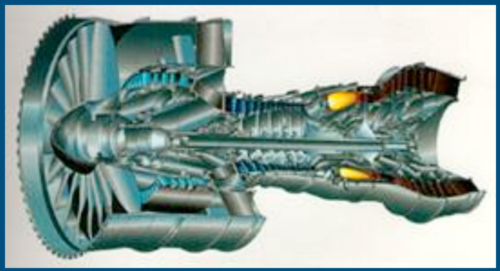
Tony Mezzacappa, Oak Ridge National Laboratory

Energy security through combustion insight

Impact: Increase thermal efficiency and decrease emissions in new land-based natural gas turbine designs

Problem:

- Understand the flamelet and thin-reaction zones where lean premixed combustion occurs
- Characterized by strong turbulence and chemistry interactions

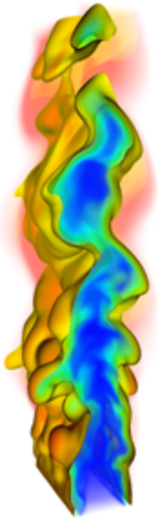


Challenges:

- Combustion at the lean flammability limit is hard
  - Prone to extinction
  - Unburned hydrocarbon emission
  - Large-amplitude pressure oscillations
  - Emission of toxic carbon monoxide

Results:

- Flame structure penetrated by small-scale eddies, but mean reaction rates still resemble a strained laminar flame



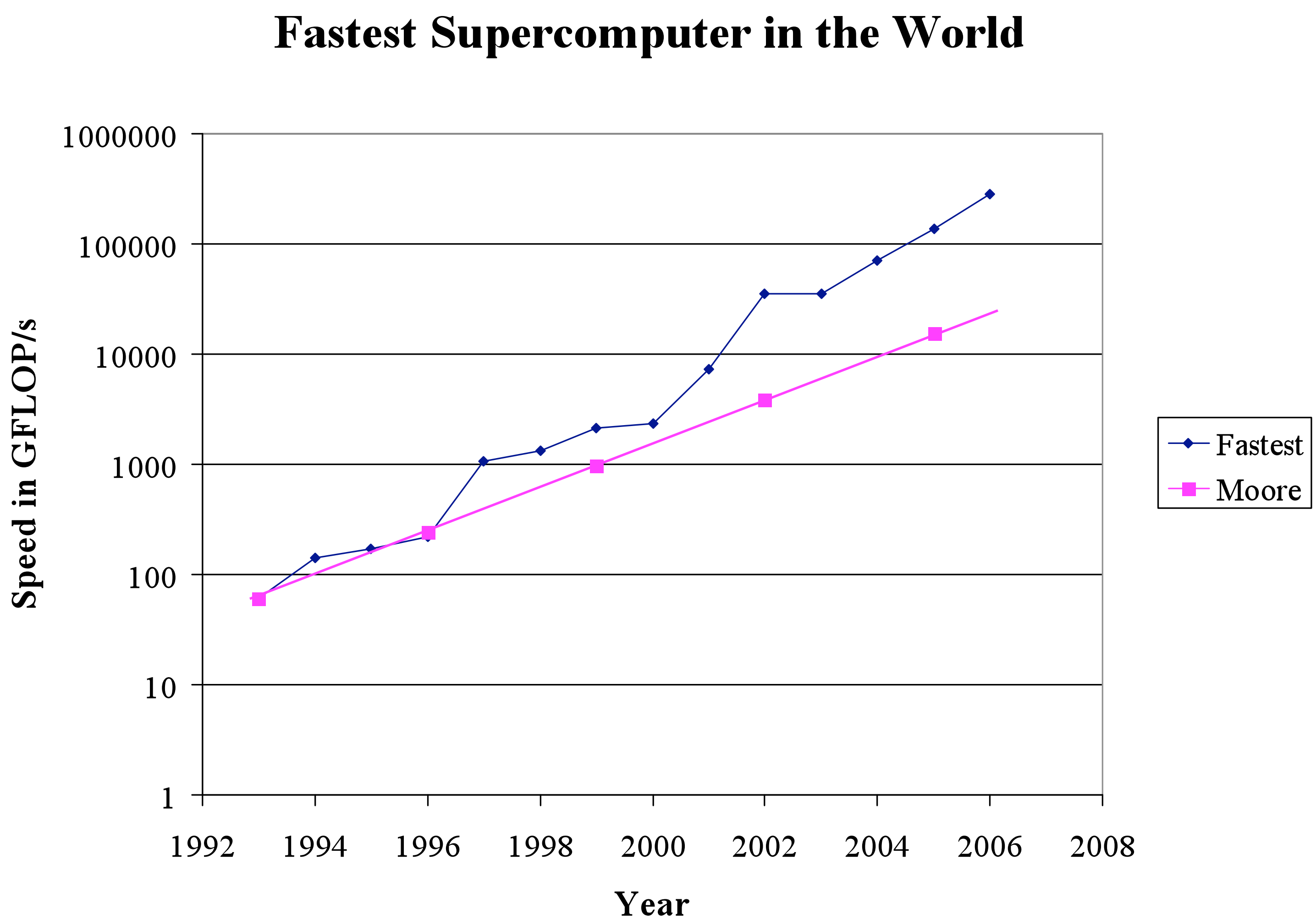
- New insights into source terms that influence flame thickness

Jackie Chen,
Sandia National Laboratories

Industry is getting into HPC

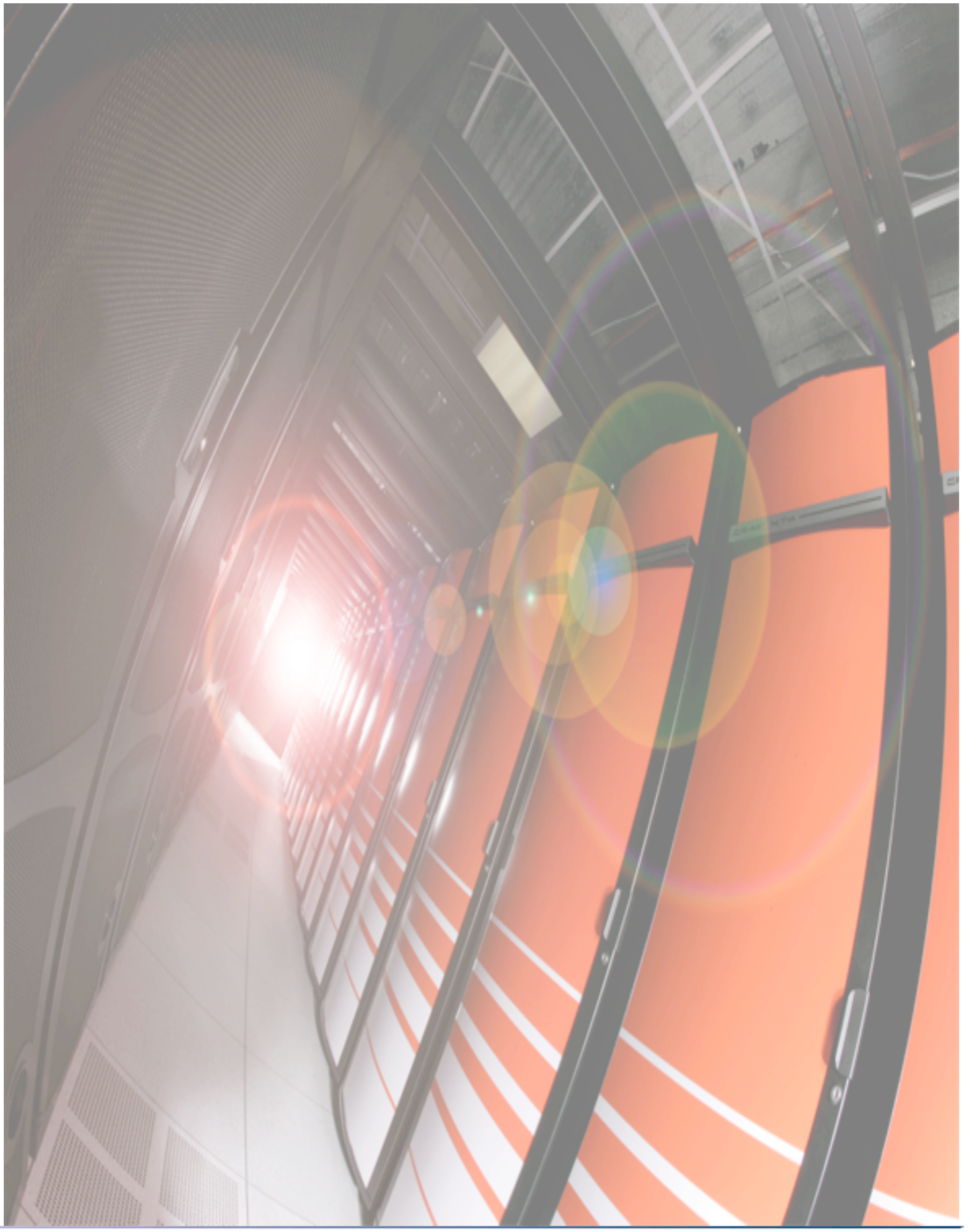
Boeing Engineering physics: Large-scale computational tools for flight vehicles	**Corning** Materials sciences: Calculation of realistic transition ranges for silica and silicate glasses
General Atomics Fusion energy: Plasma turbulence	**Dreamworks Animation** Computer science: Ray tracing

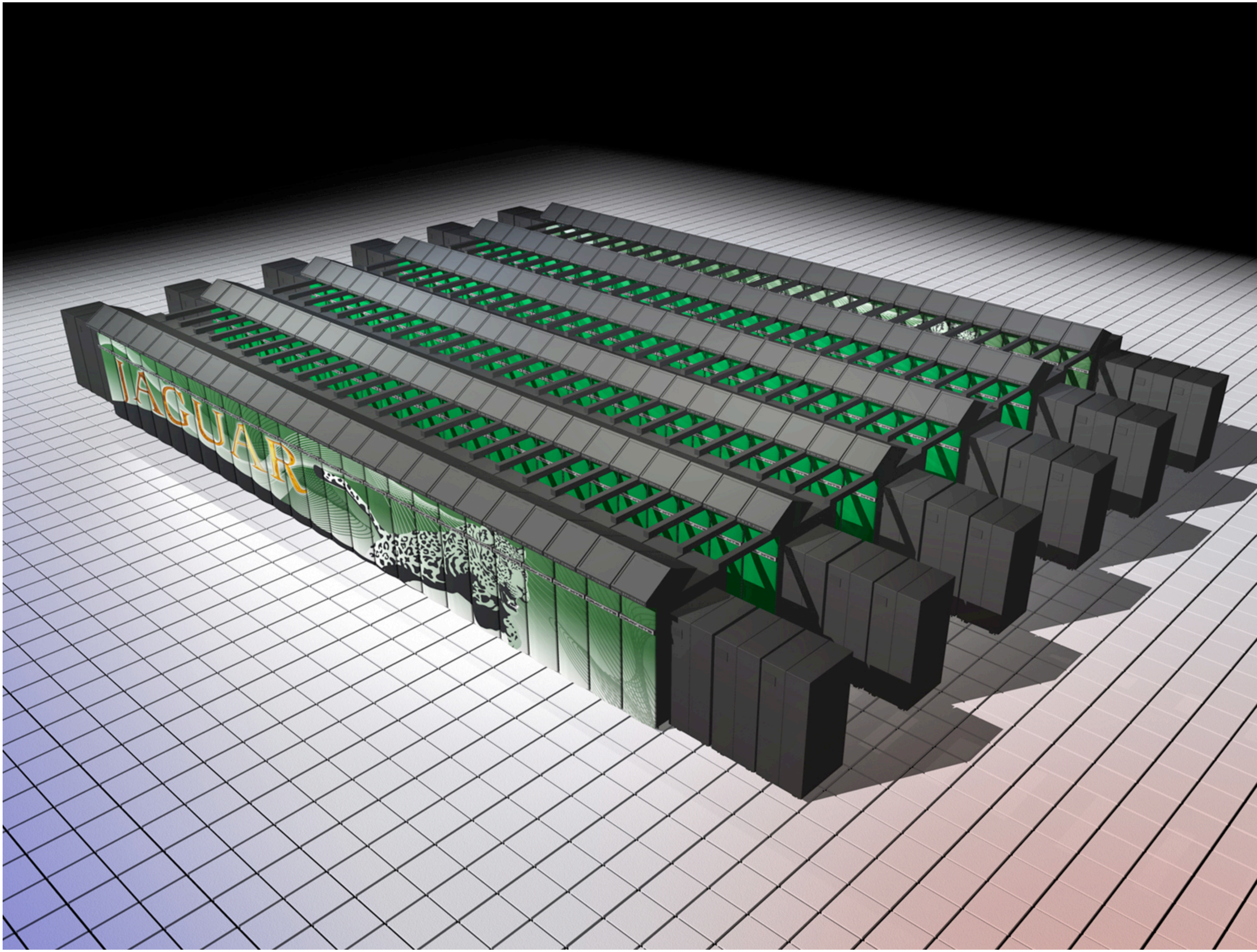
Moore's Law and Supercomputers



Jaguar - Cray XT4

- 7,832 Nodes
- 2.1Ghz quad core AMD
- 263TF
- 62TB Main Memory
- 600TB Local Disk



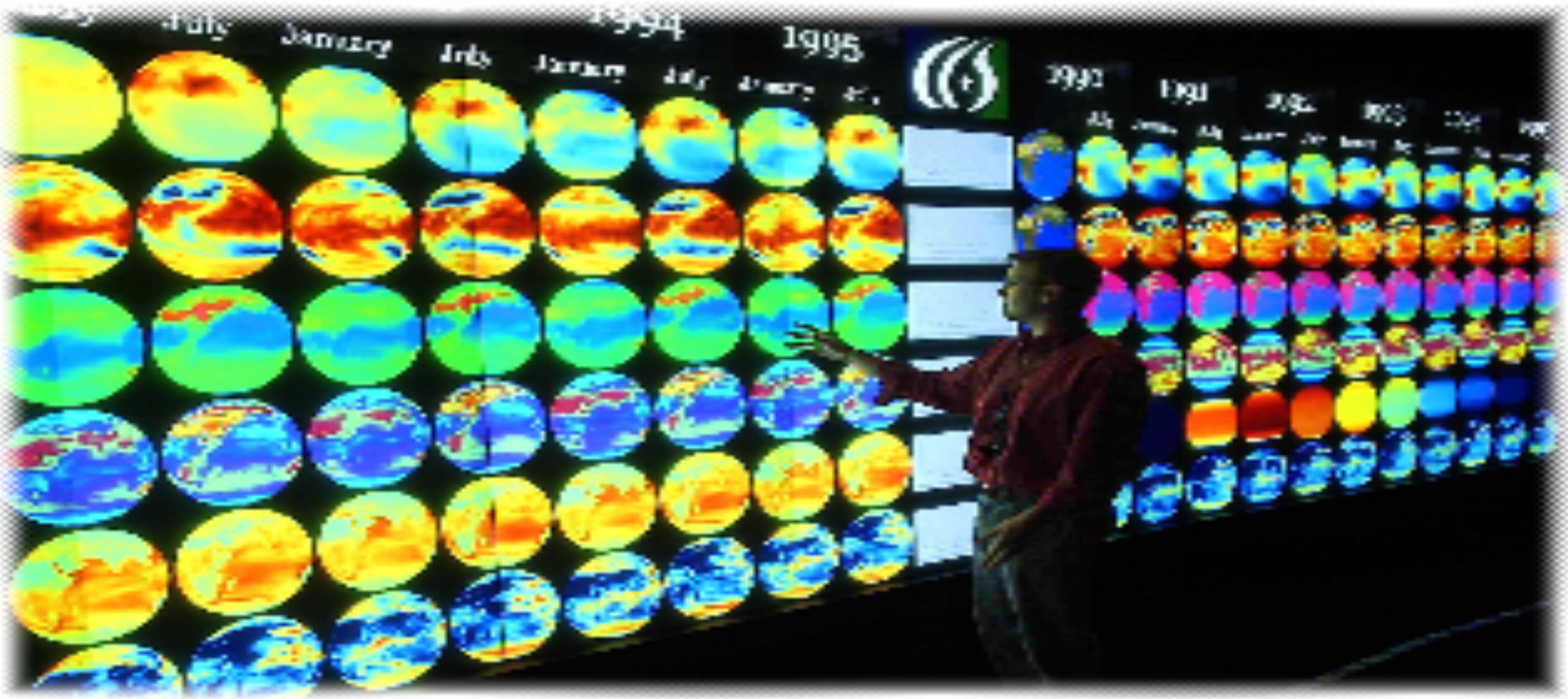

JAGUAR

Smoky

- Development cluster
- 80 nodes
- Quad-core opterons

Visualization

- 128 node Linux cluster
- 27 panel PowerWall
- 35 million pixel resolution



HPSS – Mass Storage

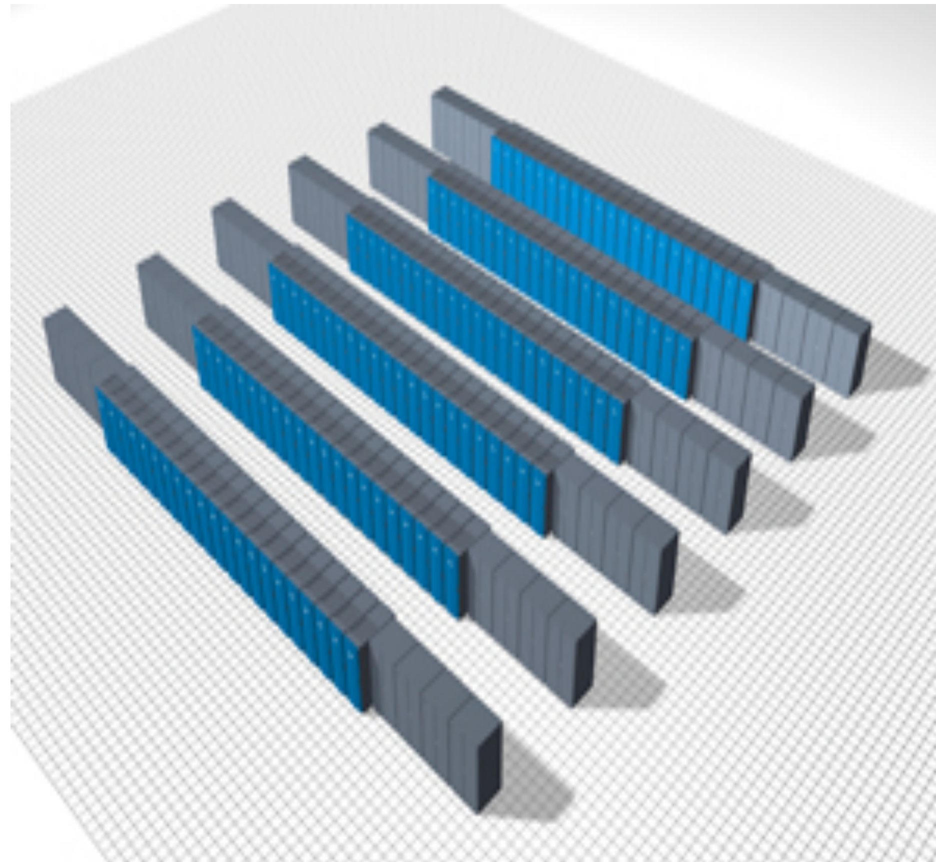
- Tape library and disk storage
- 2.5 PB stored data
- 10PB capacity
- Developer site for HPSS
- Recently expanded

National Institute for Computational Science (NICS)

- NSF Track II award
- UT/ORNL Partnership
- 170TF system in 2008
- 1PF system in 2009
- Housed at NCCS
- Managed by UT

Kraken - Cray XT4

- NICS Resource
- 170TF
- 2.2Ghz quad core AMD
- Online Summer ‘08



Course outline (subject to change)

- WEEK 1 - Course introduction
- WEEK 2 & 3 – Introduction to Unix/Linux
- WEEK 4 & 5 – Programming basics
- WEEK 6 – TOUR OF ORNL
- WEEK 7 – Parallel programming
- WEEK 8 - MID-TERM EXAMINATION
- WEEK 9 - SPRING BREAK!
- WEEK 10 – Message Passing Interface (MPI)
- WEEK 11 – OpenMP
- WEEK 12 – Model Design
- WEEK 12 – Parallel Input/Output
- WEEK 13 – Visualization
- WEEK 14 – TOUR OF ORNL
- WEEK 15 – FINAL EXAMINATION

Homework!!!!

- Send me an email
  - whittenrm1@ornl.gov
  - In subject line include [hpcc] so I can sort it
- Tell me about yourself in the email
  - Name
  - Email
  - What you'd like to get out of the class
  - Something interesting about yourself

Questions?

http://www.nccs.gov